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M.G. Lagally

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14. ABSTRACT

In this grant we concentrated on processing that makes Group IV nanomembranes viable candidates for future thermoelectric materials. In that sense, the work has been very fundamental and foundation building. The work involved using strain engineering to create new properties, especially local nano-range strain in ribbons; the integration of membranes of different orientation and composition to make a single hybrid membrane; the fabrication of massively parallel nanowires; calculations of minibands corresponding to periodic local stress distributions that create a strain heterojunction and thus a single-element electronic superlattice; and measurements of band splitting and motion with strain and initial phonon and thermoelectric measurements. We also participated in characterizing 3D nanostructures made from membranes and are going forward exploring these properties. We published 19 papers and filed two patent applications.

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Final Report

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Subject: Final Report to Dr. Gernot Pomrenke

Contract/Grant Title: Thermoelectrics Using Massively Scalable Si Nanowires

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Accomplishment Summary: Thermoelectric (TE) materials convert heat to electric power or move heat by application of a voltage. We have performed research on scalable silicon/silicon-germanium nanostructures, in particular, nanomembranes. Our approach allows us to extend standard silicon device processing to nanothermoelectrics, via the fabrication of complex sheets, nanowires, or nanoribbons. Nanostructures represent a tantalizing opportunity for improving thermoelectrics. We believe we have made significant progress and have transitioned the work into the MURI on Adaptive Intelligent Photonic/Electronic Systems (AIPES) using Si and Ge Nanomembranes. The initial work performed on this and a parallel grant enabled success of the MURI proposal.

In particular in this grant we concentrated on nanomembrane processing that makes Group IV nanomembranes viable candidates for future thermoelectric materials. In that sense the work has been very fundamental and foundation building. The work involved using strain engineering to create new properties, especially local nano-range strain in ribbons; the integration of membranes of different orientation and composition to make a single hybrid membrane; the fabrication of massively parallel nanowires; calculations of minibands corresponding to periodic local stress distributions that create a strain heterojunction and thus a single-element electronic superlattice; and measurements of band splitting and motion with strain and initial phonon and thermoelectric measurements. We also participated in 3D nanostructures made from membranes and are going forward exploring these properties. We published almost 20 papers and field two patent applications

Archival publications (published) with support of this grant:

1. Hao-Chih Yuan, M. M. Roberts, P.P. Zhang, B.-N. Park, L. J. Klein, D. E. Savage, F. S. Flack, Z.Q. Ma, P. G. Evans, M. A. Eriksson, G. K. Celler, and M. G. Lagally, "Silicon-Based Nanomembrane Materials: The Ultimate in Strain Engineering", Digest of Papers, 2006 Topical Meeting on Si Monolithic Integrated Circuits in RF Systems (SiRF06), ed. R. Drayton, IEEE, Piscataway, NJ (2006).

2. "Electrical Conductivity in Silicon Nanomembranes", P.P. Zhang, E. P. Nordberg, B.-N. Park, G. K. Celler, I. Knezevic, P.G. Evans, M. A. Eriksson and M. G. Lagally, New Journal of Physics **8**, 200 (2006).

3. "Scanning Tunnelling Microscopy of Ultra-thin Silicon-on-Insulator", P. P. Zhang, E. Tevaarwerk, B. N. Park, D. E. Savage, G. Celler, I. Knezevic, P. G. Evans, M. A. Eriksson, and M. G. Lagally, Proceedings of the 14th International Conference on Nonequilibrium Carrier

Dynamics in Semiconductors, M. Saraniti and U. Ravaioli, eds., Chicago, IL USA, July 25-19, 2005, pp. 341, Springer Proceedings in Physics **110**, 341 (2006).

4. "Silicon Nanomembranes", M.G. Lagally, MRS Bulletin **32**, 57 (2007). (invited)

5. "Elastically Strain Sharing Nanomembranes: Flexible and Transferable Strained Silicon and Silicon-Germanium Alloys", S. A. Scott and M. G. Lagally, J. Phys. D. (Applied Physics) **40**, R1 (2007) (review).

6. "Strained Si-based Nanomembrane Materials", S. A. Scott, M. M. Roberts, D. E. Savage, and M. G. Lagally, MRS Proceedings **958**, L04-07 (2007). (invited)

7. "Routes Toward Lateral Self-Organization of Quantum Dots: The Model System SiGe on Si(001)", Chr. Teichert and M.G. Lagally, Ch.2 in Lateral Alignment of Epitaxial Quantum Dots, ed. Oliver G. Schmidt, Springer Series on Nanoscience and Technology 2007

8. "Directed Self-Assembly of Quantum Dots by Local Chemical Potential Control via Strain Engineering on Patterned Substrates", M-H Huang, Feng Liu, and M. G. Lagally, in Lateral Alignment of Epitaxial Quantum Dots, ed. Oliver G. Schmidt, Springer Series on Nanoscience and Technology 2007.

9. "X-ray Absorption Spectroscopy of Strained-Si Nanomembranes", C. Euaruksakul, Z. Li, D. E. Savage, and M. G. Lagally, ECS Transactions 6, 257 (2007).

10. "A Novel Method to Fabricate Multiple-Layer SOI: Single-Crystal Si Nanomembrane Transfer and Stacking," Weina Peng, M. M. Roberts, E. P. Nordberg, F. S. Flack, P. E. Colavita, R. J. Hamers, D. E. Savage, M. G. Lagally, and M A. Eriksson, ECS Transactions 6, 333 (2007).

11. "Silicon Nanomembranes Incorporating Strain and Mixed Crystal Orientations", S.A. Scott, D.M. Cottrill, D.E. Savage, and M.G. Lagally, ECS Transactions 16, 215 (2008).

12. "Excitation of Longitudinal and Transverse Coherent Acoustic Phonons in Nanometer Free-Standing Films of (001)-Si", M. Harb, W. Peng, G. Sciaini, Ch.T. Hebeisen, R. Ernstorfer, M.A. Eriksson, M.G. Lagally, S. G. Kruglik, and R. J. D. Miller, Phys. Rev. B79, 0194301 (2009).

13. "Nanomechanical Architectures --- Mechanics-Driven Fabrication Based on Crystalline Membranes", Feng Liu, M. G. Lagally, and Ji Zang, MRS Bulletin 34, 190 (2009).(invited)

14. "Mechano-electronic Superlattices in Silicon Nanomembranes", Minghuang Huang, C. S. Ritz, B. Novakovic, D.C. Yu, Yu Zhang, F. Flack, D. E. Savage, I. Knezevic, P. G. Evans, F. Liu, and M. G. Lagally, ACS Nano 3, 721 (2009).

15. “Relationships between strain and band structure in Si(001) and Si(110) nanomembranes”, C. Euaruksakul, F. Chen, B. Tanto, C. S. Ritz, D. M. Paskiewicz, F. J. Himpsel, D. E. Savage, Zheng Liu, Yugui Yao, Feng Liu, and M. G. Lagally, Phys. Rev. B80, 115323 (2009).

16. “Semiconductors Turn Soft: Inorganic Nanomembranes”, Francesca Cavallo and M. G. Lagally, Soft Matter 6, 439 - 455 (2010) (invited).

1. “SEMICONDUCTOR NANOWIRE THERMOELECTRIC MATERIALS AND DEVICES, AND PROCESSES FOR PRODUCING SAME”, C. Ritz, P.G. Evans, and M.G. Lagally, #P06453US, filed May 7, 2007.
2. “NANOMEMBRANE STRUCTURES HAVING MIXED CRYSTALLINE ORIENTATIONS AND COMPOSITIONS”, Shelley Scott, D.E. Savage, and M.G. Lagally, June 2007, filed March 2008

Major Research Findings:

1. Nanomembrane strain engineering

$Si_{1-x}Ge_x$ with proper composition (x) was epitaxially grown on SOI, followed by a Si layer growth with a thickness equal to that of the SOI template Si layer. The SiGe layer sandwiched by the two Si layers is compressively strained due to lattice mismatch between Si and SiGe. The BOX was then removed to release the multi-layer nanomembranes. Upon release, the compressive strain in the SiGe layer was partially transferred to the two Si layers, creating elastic strain sharing between the SiGe and Si layers. The released Si/SiGe/Si nanomembranes can be transferred to any new host substrate in a similar way to that used for Si nanomembranes.

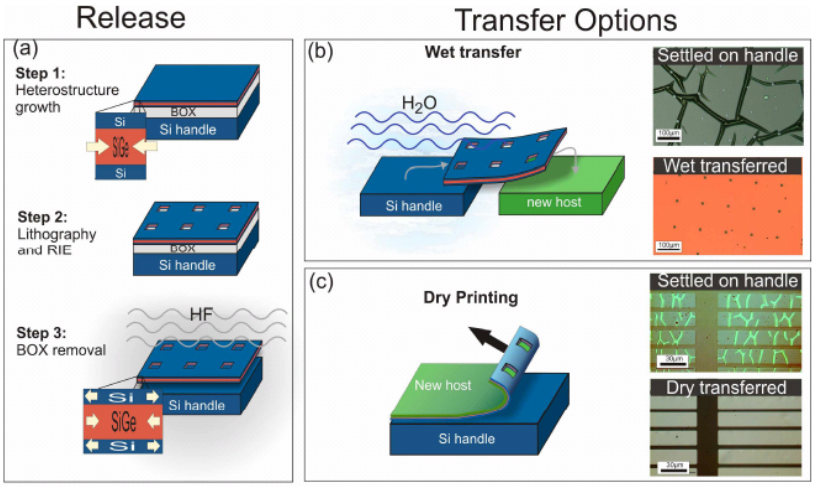

Figure 1. Strained-Si nanomembrane fabrication and transfer options

2. Local strain engineering and single-element electronic heterojunction

Single-crystal SINMs with nanometer thicknesses have mechanical properties that can be exploited to produce unique structural and electronic effects. Their mechanical compliance makes membranes fundamentally different from bulk materials or supported thin films. The growth of nanostressors on ultrathin Si membranes takes advantage of this mechanical com-

pliance to create a “strain lattice” consisting of very small regions of high local strain in the membrane, the order occurring because the local strain provides a strong and precise feedback for self-organization of the nanostressors. The strain lattice in the Si membrane in turn produces a modulation in the electronic band structure that extends through the thickness of the membrane and thus creates an electronic superlattice without a need for compositional modulation, the conventional method for forming electronic heterostructures. The ability to create straightforwardly such functional superlattices in semiconductors has significant implications for the development of nanoscale photonic, electronic, and thermoelectronic devices. The mechanism should be accessible in membranes of all the semiconductor systems that exhibit strain-mediated growth of nanostructures.

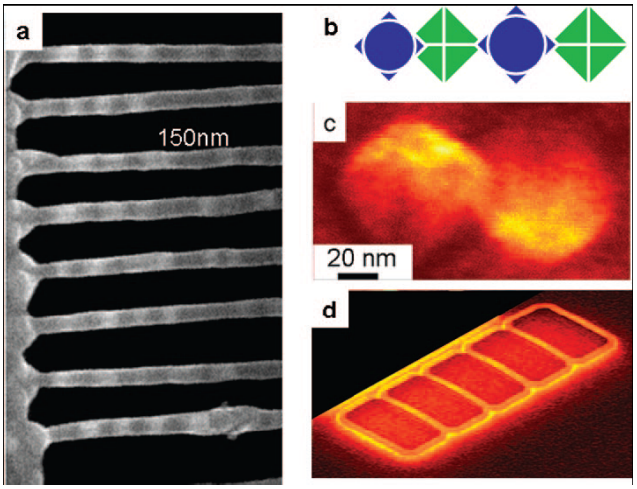

Figure 2. Si nanoribbons with periodic Ge nanostressors. The Ge nanostressors form on opposite side of the ribbon in a periodic fashion. a) SEM of ribbons with Ge dots. b) schematic diagram of dots forming on opposite sides. c) Colorized SEM image of two dots on opposite sides of the thin SiNM. d) larger-scale colorized SEM image of a ribbon array.

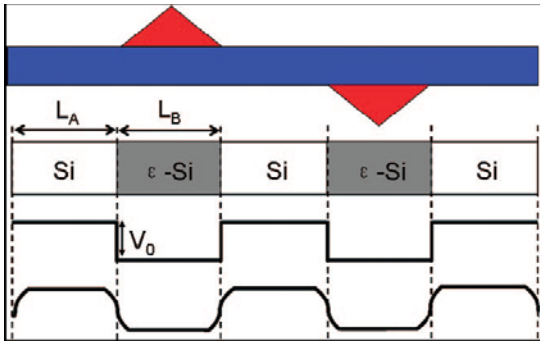

Figure 3. Schematic diagram of the structure and potential energy diagram for the strain superlattice. The band offset is 80% in the conduction band, allowing us to a create Kronig-Penney model to describe the 1D potential along the ribbon. The bottom diagram is used in detailed calculations of miniband formation. Band offsets, V_0, can be as much as 200 meV.

3. *Relationships between strain and band structure in Si nanomembranes*

The flexibility of single-crystal Si nanomembranes allows strain to be applied elastically without introducing dislocations in the fabrication process, resulting in uniform strain. It is also relatively easier to apply different types and orientations of strain to Si using elastic-strain sharing than by the traditional graded-strained-layer approach. We use X-ray absorption spectroscopy to measure the effect of uniform biaxial strain on several features of the conduction band structure of Si with (001) and (110) orientations. By also measuring the Si 2*p* photoelectric threshold, we are able to determine the absolute positions of features of the Si conduction band and their change with strain. This result is important because it allows us to determine for given values of strain what the band offset is that we use above in the periodic single-element electronic superlattice.

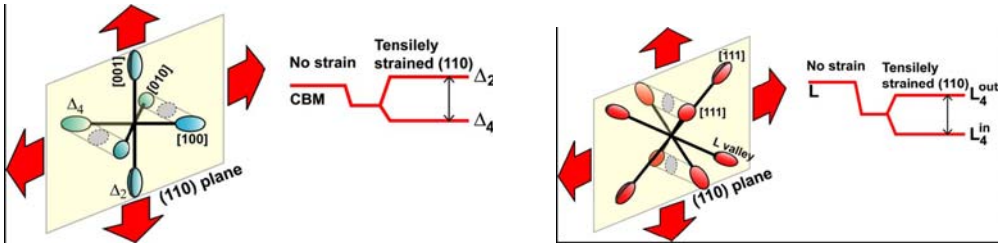

Figure 4. Schematic diagrams of conduction band minimum shifts in Si(001) (left) and Si(110) (right).

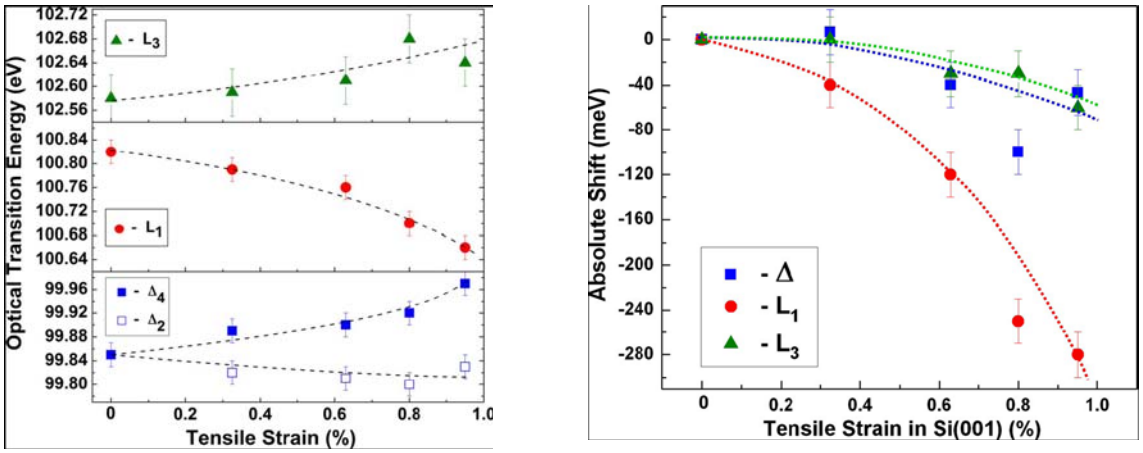

Figure 5. Relative and absolute energy shifts with tensile strain of several valleys in the conduction band of Si(001). Note that different valleys move by different amounts for a given value of strain.

4. *Silicon Nanomembranes Incorporating Mixed Crystal Orientations*

We have developed initial processes for fabricating mixed-crystal-orientation nanomembranes or equivalently mixed composition nanomembranes, using Si nanomembrane (SiNM) transfer and overgrowth, to produce a "quilt" of Si(001) and Si(110). The selective growth of Si(001) compared to Si(110) in CVD growth has been used to planarize hybrid-orientation surfaces, formed by releasing and transferring Si(110)NMs. These features have the potential to be of use on a variety of different host surfaces because of the possibility of transfer. We use the same sorts of transfer processes described earlier but add her selective growth via CVD

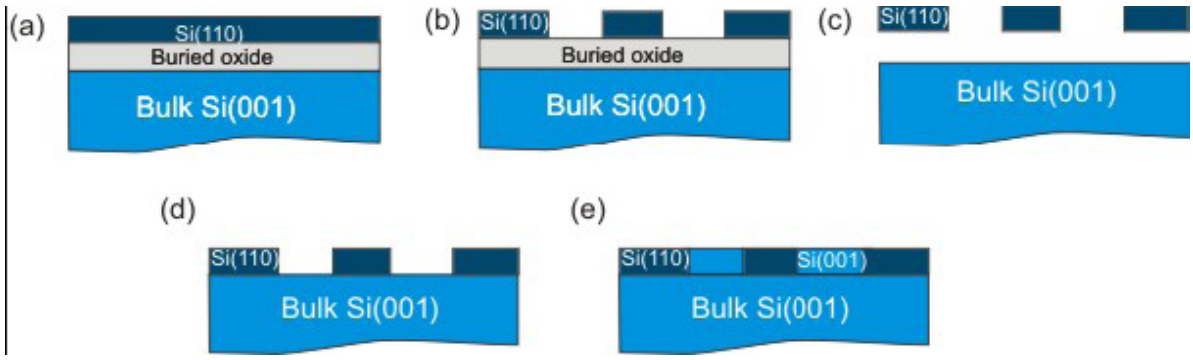

Figure 6. HOT fabrication via membrane transfer and overgrowth, illustrated in cross section. (a) The original SOI(110) substrate; (b) after lithography and RIE; (c) after removal of the buried oxide in HF; (d) after bonding to a bulk Si(001) substrate; (e) after CVD growth of Si.

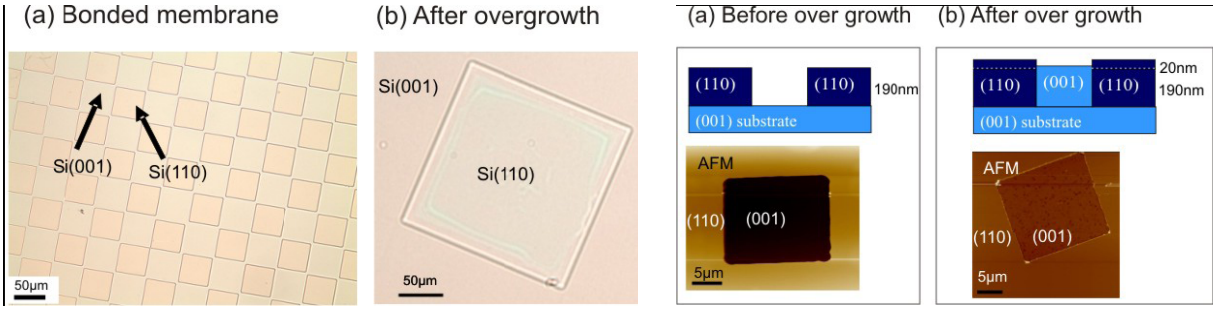

Figure 7. Images of Si(001) and Si(110) HOT structures, both before and after filling of the holes in the covering membranes by selective growth.